1,1,2,3-Tetrachloropropene

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Model Performance

Model Data	
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 4.45

Global applicability domain: Inside

Local applicability domain index: 9.88e-01

Confidence level: 6.40e-01

Nearest Neighbors from the Training Set

Image not found

1,3-Dichlorobenzene

Measured: 4.12 Predicted: 4.44 Image not found

1,4-Dichlorobenzene

Measured: 4.46 Predicted: 4.45

Image not found

1,2-Dichlorobenzene

Measured: 4.36 Predicted: 4.46

Image not found

Propylbenzene Measured: 4.09 Predicted: 4.53 Image not found

Octanal

Measured: 5.36 Predicted: 4.54